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Modeling of Building Scale Flow and Dispersion

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1. INTRODUCTION

Predictions of airflows around buildings and the associated thermal and dispersion phenomena continue to be challenging because of the presence of extremely heterogeneous surface structures within urban areas. Atmospheric conditions can induce local winds to flow around structures rather than over them. Thus pollutants that are released at or near the ground tend to persist at relatively low levels with only minimal ventilation of the airborne material away from the ground surface. While flow and dispersion phenomena can be studied within wind tunnel settings, recent advances in numerical modeling have enabled computational fluid dynamics (CFD) to evolve into an important tool in the simulation of building scale flows. We are developing numerical models to simulate the flow and dispersion of releases around multi-building complexes. These models will be used to assess the transport and fate of releases of hazardous agents within urban areas and to support emergency response activities.

There are already a number of models that have been developed to simulate flow and dispersion around urban settings. A recent collection of these papers can be found in the Proceedings of the International Workshop on CFD for Wind Climate in Cities[1]. Most of the simulation studies presented in the literature are based on single buildings with a few of these results compared with wind tunnel experiments. As the applications become more advanced, the influence of multiple buildings, vegetation, surface heating and atmospheric stability on flow and dispersion has begun to be incorporated into recent CFD models.

The focus of this paper is to describe LLNL's effort in the development of a high-performance CFD model for simulating transport and diffusion of hazardous releases around buildings and building complexes. A number of new physics features have been implemented in order to customize our CFD model for the urban application. These include surface heating, vegetation canopy, heat and mass transfer, and atmospheric stratification. Among the other issues considered are ingestion of urban databases, grid nesting (coupling with larger scale meteorological models), assimilation of meteorological or gridded data, and initial and boundary conditions.

Examples to support the discussions will be drawn from modeling studies that have been conducted, in part, to validate simulated results with laboratory (wind tunnel) and field experiments.

2 The CFD model (FEM3MP)

FEM3MP is a third-generation adaptation of the $FEM3C^2$ model that was developed to simulate flow and dispersion of heavier-than-air gases. The current model is a high performance (massive-parallel) version of the model and includes several new features that are specific to the building dispersion application. The model equations and a detailed description of this model can be found in Chan and Lee.[6] Some relevant aspects of the model are:

- Finite-element technique
- Fully 3-D
- Use of projection method and fully implicit time integration scheme
- Generalized anelastic formulation
- Explicit treatment of terrain and surface obstructions
- Option of several Reynolds-averaged Navier-Stokes (RANS) turbulence submodels or a Large Eddy Simulation (LES) model
- Explict urban physics such as surface heating (including shadowing), tree canopy, and aerosol physics

FEM3MP uses a modified finite element technique to provide great flexibility in the arbitrary grading of the mesh in order to economize on computational costs. While the standard Galerkin finite element formulation can be easily applied to very general meshes, it is also computationally expensive to use. In FEM3MP we employ a number of simplifications to the traditional finite element method to permit the code to be computationally affordable for three-dimensional problems.

Rather than solving the coupled set of momentum and continuity equations, the model uses a segregated approach in which the system is decoupled by using a consistent pressure Poisson equation in lieu of the continuity equation. This projection method was first proposed and analyzed by Chorin[7] and many variants of this algorithm have been used in the computation of incompressible flows. Some key features that contribute to the computational efficiency of the model include:

- Logical (i, j, k) but non-uniform grid system
- Choice of a highly efficient conjugate gradient pressure solver or a multigrid solver
- Fully implicit time integration treatment for diffusion and linearized implicit treatment for advection

There are options for three different RANS turbulence formulations in FEM3MP. They range from the simplest K-Theory, two-equation (k-ε), to an advanced three-equation (k-ε-A_2), where A_2 is the second invariant of the anisotropic part of the Reynolds stress tensor. Although more computationally expensive than the first two formulations, the three-equation model has the advantage that wall functions are not needed since the viscous surface layer can be computed directly.

The boundary conditions used in the model are typically a combination of Dirichlet (specified velocity and temperature) or specified normal and tangential stresses and heat flux. At the outflow, "natural" (zero stress and heat flux) boundary conditions appear to work well except for the most difficult simulations.

Pollutant sources are modeled either as a puff (limited time duration) or as continuous releases. In the Euler representation, point sources are distributed over a few, highly graded, mesh cells with the spatially integrated pollutant mass flux equal to the required source strength. If the flow is steady-state and the pollutants of current interest are assumed to be inert, concentration calculations can be performed from a velocity field that has been computed ahead of time. For highly transient flows, such as those resulting from LES simulations, concentrations calculations are computed simultaneously with the flow field.

3. URBAN DISPERSION MODELING SCALES AND GRID NESTING

Analysis of airflow and dispersion for urban settings involves three distinct scales of interest:

(a) *Single to few buildings scale* –This scale focuses on highly resolved simulations around a single building or a building complex involving several buildings with domain size of one to a few kilometers and dispersion time scales on the order of minutes.
(b) Many building scale – Only clusters of buildings, rather than individual buildings, can be resolved within this scale. Typical domain sizes for this case are tens of kilometers and dispersion time scales of one or a few hours.
(c) Urban/regional scale – The urban scale encompasses the entire urban and suburban area, reaching the lower spatial limits of a typical regional weather forecast. Domain sizes represented are of order 100 kilometers and up and dispersion times scales of several to many hours. Buildings can no longer be resolved under this coarse spatial resolution thus their effects have to be parameterized.

CFD calculations are performed within limited area domains that are typically driven by boundary and initial conditions from large-scale forecasts. Grid nesting techniques have been used in many models to interface meteorological data between varying domain sizes and grid resolutions. Building scale simulations are particularly challenging for grid nesting because of the difficulty in representing building interactions between grids via boundary conditions. In FEM3MP we use a combination of "sponge" and "nudging" lateral boundary conditions to transition between nests.

4. MODEL SIMULATIONS

4.1 Wind Tunnel Dispersion Study

LLNL and LANL, via support from the Department of Energy's Chemical Biological National Security Program (CBNP), jointly contracted with NOAA to conduct wind tunnel experiments at the EPA's Fluid Modeling Facility. These experiments were focused on the physical modeling of flow and dispersion of releases within multiple block arrangements with the data being used for validation studies. The experiments involve both 2D (rectangular blocks) and 3D (cubicles) configurations of obstacles as a crude representation of buildings. Detailed measurements of mean flow, turbulence and concentrations from source releases were made in order to compare with the CFD simulations. Figure 1 depicts the resulting flow vector and turbulent kinetic energy (tke) fields for the 3-dimensional 7 x 11 block configuration. Results from RANS and LES simulation

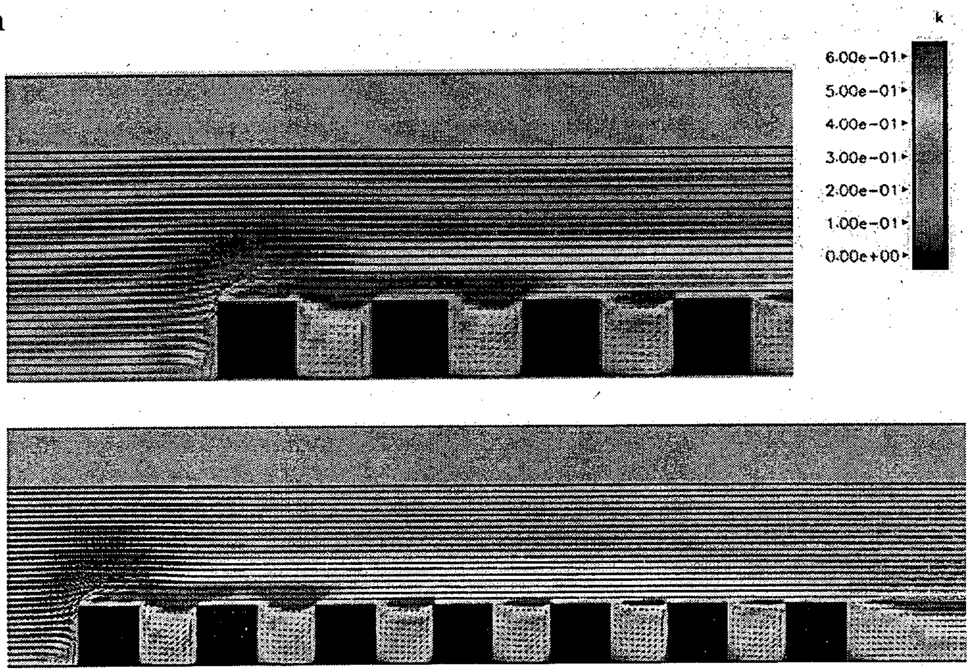

Figure 1: Velocity vectors and tke field for flow around multiple blocks in a wind tunnel

4.2 *Flow around a single building*

Our CFD model has been used to simulate the wind field and dispersion of releases around a complex, but isolated, building at LLNL. The results were compared with field data taken around the particular building over an intense observational period in the summer of 1999. CFD calculations were performed before the field experiments in order to guide the placement of wind sensors and to locate "hotspots" where the flow dynamics were particularly interesting. Among the most interesting aspects of the simulation are the complexity of the geometry of the two-level building and the convergence/divergence of the flow due to the row of tall trees adjacent to the building. Figure 2 shows comparisons between the simulated and observed winds at various locations about 2 meters above ground level. The darker shaded area denote regions of low wind speed caused by the flow obstruction by the building and the trees. Model results agreed well with data except for the low speed recirculation zones adjacent to the building where the wind directions were highly variable and less well-defined.

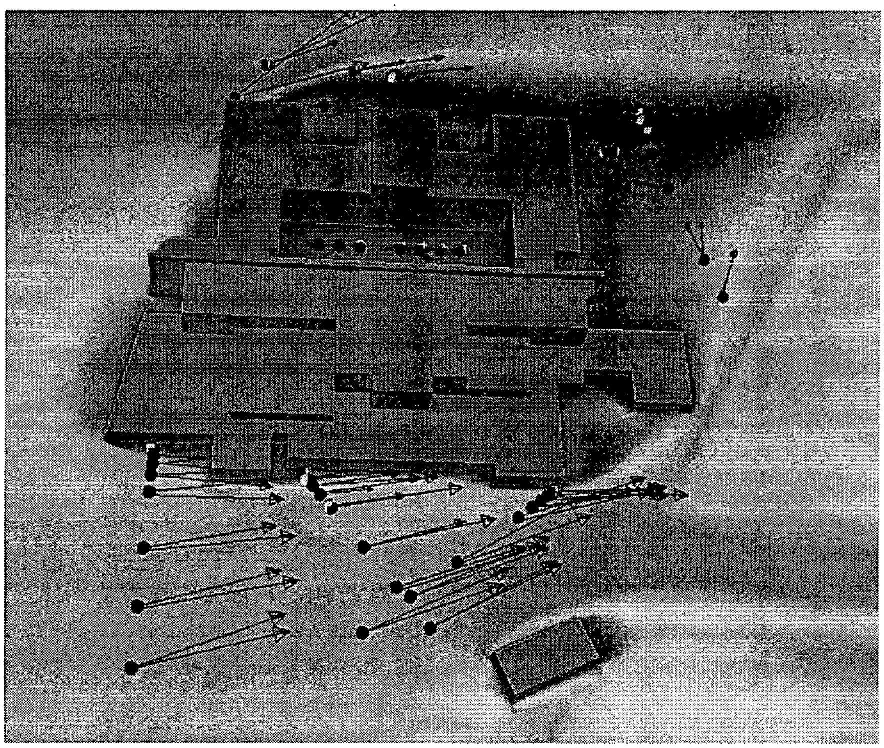

Figure 2: Simulation of flow around a complex single building – comparison of model results with field data

4.3 *Flow and dispersion within an urban area*

DOE's CBNP supported an extensive field experiment campaign in the Fall of 1999 to collect data related to the atmospheric flow and dispersion around the downtown Salt Lake City area. Among the data that were available included surface measurements as well as vertical profiles of winds and temperature from in-situ and remote sensing instruments. In addition to meteorological data, the experimental team also conducted tracer experiments near a particular building with the associated dispersion pattern determined by a network of concentration measurement samplers.

As for the LLNL single building study, our CFD model performed a number of simulations to guide the selection of a release location and to assist in the planning of where to place wind and concentration samplers. The simulated domain is a section of downtown within a 2 km x 2 km area containing about 500 buildings. Figure 3 shows a simulated concentration isosurface from a release in front of a building where the actual source was located. It is noteworthy that, since the experiments were performed at night, terrain-induced drainage flows came into play on a larger scale. These intermediate scale flows can be incorporated by nesting the building scale calculations within a larger domain which included the mountains east of the Salt Lake basin.

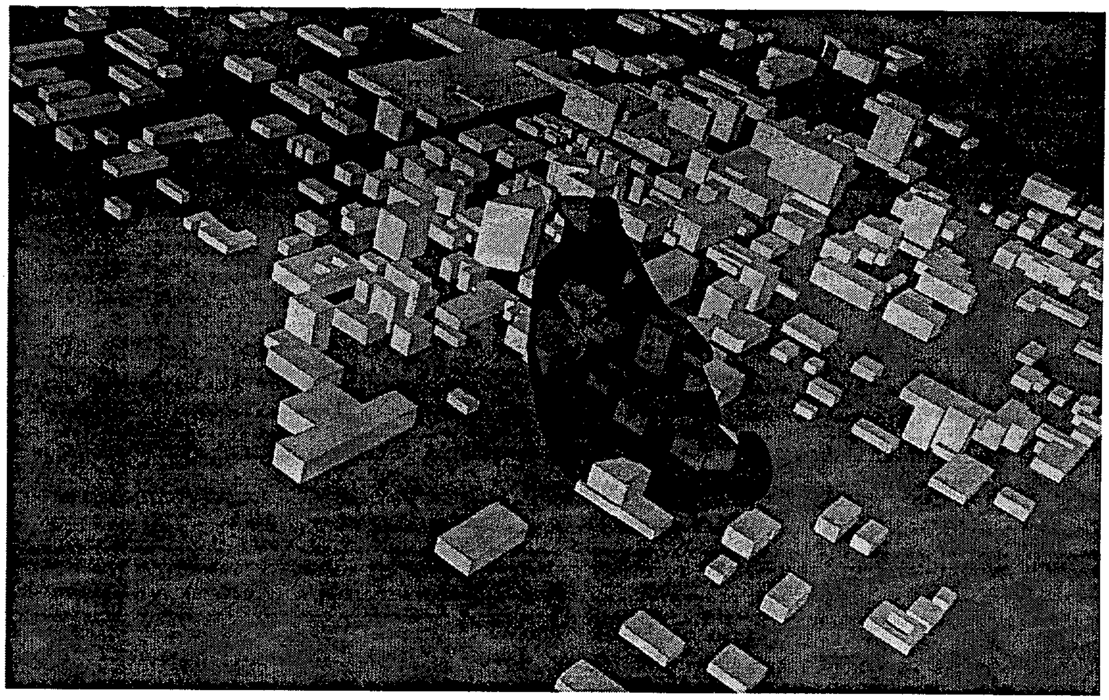

Figure 3: Dispersion of a release within an urban downtown area

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